

A. Professional Preparation:

Birla Institute of Technology and Science, India	1977 MSc (Hons)
The Johns Hopkins University	1981 M.A. & PhD
Post-doc, Lawrence Berkeley Lab	
University of California, Berkeley	1980-1983

B. Appointments: Lawrence Livermore National Laboratory, and , Lawrence Berkeley National Laboratory, UC Berkeley, Senior Scientist 2000-
Adjunct Professor, Dept. of Mathematics & Computer Science, California State University, Hayward, CA 2003
University of California (UC), Davis, Department of Applied Science,

Step VI Professor 2000-2003

Arizona State University

Professor Emeritus 2000-

Professor 1990-2000

Associate Professor 1987-1989

Assistant Professor 1983-1986

Distinguished Professor, Indian Institute of Science, Bangalore, India Spring 1997

Honors and Awards

Elected Member of [International Academy of Mathematical Chemistry](#) 2004

National Academy of Sciences, Advisory Panelist

Chemistry and Materials Science Directorate Associate Director Award, Exceptional Service Award, Recipient of the distinguished 2003 Robert S. Mulliken Award 2003

IIT Madras, Director Extramural Distinguished Lecture

Joint Prize of Minister of Education, Polish Government 1998

Top 0.1% of most cited Chemists 1986-1997

Fulbright Distinguished Professor Research Award 1996-1997

Award for Distinction in Graduate Teaching 1991

The Camille and Henry Dreyfus Teacher-Scholar Award 1985-1990

Birla Institute of Technology & Science Distinguished Lecturer & Alumnus Award 1989

Alfred P. Sloan Fellow 1984-1988

Citation from Institute of Scientific Information as the author of one of most cited 1986 Chemistry papers

National Science Talent Scholar 1973

Editorship

Mathematical & Computational Chemistry

Editorial Advisory Board

[Journal of Mathematical Chemistry](#)

[Journal of Zhejiang University Science](#)

[Journal of Computing Letters](#)

Scientific Panels

Advisory Panel to the Chemical Sciences Division of the Air Force Office of Scientific Research, DOE panel for the Laboratory Technology Program, DOE Environmental Management Science Program (EMSP) Panel, NSF panelist, DOE-BES Panelist

Research Interests

Computational nanotechnology, Development of Engineered mesoporous materials for sensors, Computational biotechnology, Machine Learning, Artificial Intelligence, Graphs, Discrete Math & Applied Computer Science, Computational Actinide chemistry with applications to energy and environment, Catalysis, Energy Conversion and Hydrogen Storage, superheavy molecules, bioinformatics, relativistic electronic structure, and chemical applications of graph theory.

Recent Research Grants

- 1. Engineered Mesoporous Materials for the development of Actinide Detection, Sequestration & Sensors, Department of Homeland Security, \$170,000 for FY2012 \$1560,000 from 2008-2011 and a Continuing multi-year Grant.**
- 2. Electronic Structure of Transition Metal Clusters & Reactivity, and Electronic Structure of Environmental Actinide Complexes, \$241,000 for FY2011-2012 , \$122,000/ FY2013 and a Continuing multi-year Grant since 1986 with an unprecedented repeat record of renewals continuously from 1986, US Department of Energy, Office of Basic Energy Sciences, Washington, DC**

Publications

600+ Journal Publications, 2 John Wiley Book, 22 Chapters in Books

See attached for the list for some of the publications